Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Electronic origin of spin phonon coupling effect in transition-metal perovskite materials HONGWEI WANG, Temple University, LIXIN HE, University of Science and Technology of China, HONG JIANG, Peking University, XIFAN WU, Temple University — Spin-phonon couping in transition metal ABO_3 perovskites can be identified by the softening of the low-lying phonon modes including the polar ones, when the spin configuration is changed from being antiferromagnetic (AFM) to being ferromagnetic (FM). We studied the spin-phonon coupling effect by computing the changes of the superexchange energies as functions of typical soft modes' amplitudes in $SrMnO_3$ as an example. The superexchange interactions are computed by a recently developed extended Kugel-Khomskii model based on maximally localized Wannier functions. The spin-phonon coupling effect in $SrMnO_3$ is generally attributed to the suppressed superexchange interaction by all the soft modes under investigation. However, the spin-phonon coupling strength varies significantly among all the different soft modes. The individual superexchange interaction involves the hopping process between the d-like state of neighboring metal ions with strong hybridized oxygen p character. As a result, the phonon modes, such as Slater and antiferrodistortive mode which modify the relative position of metal ion and oxygen octahedral cage, are found to be more effectively important in spin-phonon coupling effect. Furthermore, the electronic configuration also plays a crucial role.

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Date submitted: 17 Nov 2016 Electronic form version 1.4